

Dimethyl succinate

106-65-0 | DTXSID5025152

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 2.84e-01 mol/L

Global applicability domain: Inside

Local applicability domain index: 8.16e-01

Confidence level: 6.93e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Dimethyl succinate</div> <div>Measured: 1.71e-01</div> <div>Predicted: 2.84e-01</div>	<div>Image not found</div> <div>1,2-Ethanediol diacetate</div> <div>Measured: 1.22</div> <div>Predicted: 4.77e-01</div>	<div>Image not found</div> <div>Peroxide, bis(1-oxopropyl)</div> <div>Measured: 1.09e-01</div> <div>Predicted: 2.17e-01</div>
<div>Image not found</div> <div>Dimethyl maleate</div> <div>Measured: 5.55e-01</div> <div>Predicted: 3.81e-01</div>	<div>Image not found</div> <div>Dimethyl glutarate</div> <div>Measured: 3.68e-01</div> <div>Predicted: 4.48e-01</div>	